

Slowdown of nonequilibrium dynamics in gapped ‘qubit’ chains

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Abstract

We solve the nonequilibrium dynamics of qubits or quantum spin chains ($s=1/2$) modeled by an anisotropic XY Hamiltonian, when the initial condition is prepared as a spatially inhomogeneous state of the magnetization. Infinite systems are studied analytically, yielding a universal relaxation driven by quantum fluctuations. Particular long-lived excitations are found, for which the relaxation time diverges as a consequence of constructive quantum interference at degenerate stationary points. Those states are intrinsically entangled and may be of interest for performing quantum computation. We also numerically analyze finite samples to assess the extent of size effects.

1 Introduction

Magnetic quantum systems which displays a slow relaxation in the nonequilibrium dynamics are good candidates for magnetic data storage devices. Low dimensional magnetic systems, including magnetic chains and magnetic molecules in molecule-based magnets, may allow for a substantial reduction of the size of memory units to perform classical computation [1]. In addition, systems that develop quantum coherence in the nanometer scale may be of interest for the fabrication of quantum computers. Quantum computation is believed, at least in principle, to be much faster than classical computation, and its accomplishment rests in the ability of a quantum system to be in a superposition of many quantum states (*entanglement*). This property is the basis of the so called *quantum parallelism*, which presents a lot of advantages in relation to its classical counterpart, the one that is realized in a classical computer by connecting a large number of processors for parallel operation. Still, there is another important requirement for doing efficient quantum computation, a condition that is related to quantum programming or quantum software: we need robust Bell-like

states, or stable entangled states devised through constructive interference from the many quantum states available. The coherence time of those states must be much larger than the time employed in 1-qubit or 2-qubit operations [2].

The present contribution is related to this latter issue. It has been shown that quantum chains which are modeled through the Heisenberg Hamiltonian (or variants such as the quantum XY model), are intrinsically entangled [3]. The quantum XY model can be practically realized in low-capacitance Josephson junction arrays [4]; it also appears as an effective Hamiltonian for the interaction of quantum dot spins [5], and it is also relevant for other condensed matter and QED systems which have been proposed as quantum computers [2]. One important role of the XY model in quantum computation is that it can be used to construct a *swap* gate, which means that the time evolution can be considered as a source of entanglement [3]. Moreover, an interesting connection between quantum phase transitions and entanglement has been recently proposed, suggesting that entanglement plays an important role in quantum critical phenomena [6]. Concerning the anisotropic XY model, a quantum phase transition is found as a function of the anisotropy parameter and transverse field. The latter may be envisioned as a quantum metal-insulator transition with the formation of a gap for the insulating phase.

Here, we are able to construct analytic solutions of the anisotropic XY model in the thermodynamic limit, which display a very slow relaxation after being prepared in a non-homogeneous initial state. This is a peculiar nonequilibrium problem, since our quantum system is closed (does not exchange energy with the environment except when preparing the initial condition), and its relaxation to the homogeneous state is exclusively driven by quantum fluctuations and interference effects. Nonequilibrium properties of quantum systems have been recently investigated by several authors following different approaches [7, 8, 9], but a complete theory is still lacking. To test our solutions, we also study finite systems through numerical calculations. Finite systems are interesting for practical applications, like the ones mentioned above. An important question to answer is whether a finite system will show similar relaxation properties, at least during finite periods of time, and how to monitor the magnitude of such periods.

In spite that we solve a well defined model, some properties of the phenomenon seem to be universal for one dimensional systems. *The key point addressed in this paper is how to prepare special long-lived superposition states in quantum magnetic chains, whose coherence is not wiped out by the strong destructive interference that appear at very long time.* We call those states as *critical*, for reasons that will be developed in the next sections.

A general nonhomogeneous initial state in a quantum spin chain can be Fourier decomposed. We then study the nonequilibrium dynamics through the time evolution of the Fourier component of the magnetization $\langle \tilde{\mathbf{S}}_Q \rangle_t$. This approach has several advantages in spite that $\tilde{\mathbf{S}}_Q$ is not an observable: one can probe the relaxation properties as a function of the wave vector Q , which is an important parameter in the theory, and for the particular case of the XY

model (and variants), the relaxation of the longitudinal component $\langle S_Q^z \rangle_t$ is independent of the initial state, except for a complex scale factor, *i.e.*

$$\langle S_Q^z \rangle_t = \langle S_Q^z \rangle_0 f^z(Q, t), \quad (1)$$

where f^z is a real universal function that depends on parameters of the Hamiltonian. We are interested in solving the anisotropic XY magnetic chain with spin 1/2 in the presence of a transverse magnetic field

$$\mathcal{H} = 2\hbar\omega_J \sum_{j=1}^N \left\{ r S_j^z + [(1+\gamma) S_j^x S_{j+1}^x + (1-\gamma) S_j^y S_{j+1}^y] \right\}, \quad (2)$$

where $\hbar\omega_J$ is the exchange integral, $r = (\omega_0/\omega_J)$ is the external transverse field in units of the exchange constant, $0 \leq \gamma \leq 1$ is the anisotropy parameter, N is the total number of spins in the chain, and $S_j^\alpha = (1/2)\sigma_j^\alpha$ are spin 1/2 operators. Special cases of this model are:

- i) the isotropic XY model with a transverse field ($\gamma = 0$);
- ii) the Ising model with a transverse field ($\gamma = 1$);
- iii) no magnetic field ($r = 0$).

The chain is prepared in an arbitrary nonhomogeneous initial state and its magnetization dynamics is calculated in exact form under very general assumptions. In the thermodynamic limit ($N \rightarrow \infty$), and for long times, the system displays irreversibility in the form of a power law relaxation. This irreversibility can be ascribed to quantum interference effects which encompass the system at asymptotically long times. In analogy with classical optics, we handle this phenomenon using the stationary phase method [10]. As a general rule, most of the components interfere destructively (shadow regions), and the relaxation is dominated by the contribution of stationary points, where the interference is constructive (illuminated zones). It may happen that some stationary points become degenerate in the parameter space. In optics, we get surfaces where the intensity of light diverges (*caustics*). In our problem, we get critical states whose relaxation time asymptotically diverges, yielding a very slow relaxation. Those critical modes do not occur in all cases, and we present a summary of our findings below.

Models i) and ii) were discussed in Ref. [11]. Also Berim and Cabrera [12] and Berim, Berim and Cabrera [13] have solved similar problems for several versions of the 1-dimensional XY model, which include dimerization, bond alternation, and staggered magnetic field. All the models, including the one presented here, are amenable of exact analytic treatment by fermionization methods involving generalized Jordan-Wigner transformations [13, 14]. *Concerning relaxation properties, all the models studied can be grouped into two families, whether the energy spectrum has a gap or not* [13]. Only gapped models develop critical modes with anomalously slow relaxation properties. It remains

the question whether the above phenomenon is associated to a conservation law [13]. It is then interesting to study the behavior of Hamiltonian (2), since the anisotropy in the XY exchange and the transverse magnetic field lift the spin rotational symmetry and the time reversal symmetry, respectively. Moreover, one can monitor the spectral properties (gap or not) with γ and r . The present study confirms the general prescription stated in Ref. [13] for the XY family, *i.e.* anomalous long-time tails in the relaxation are features of gapped one-dimensional models. In this contribution, we will show that this anomalous slowing down of the relaxation is due to both, constructive quantum interference at degenerate or *critical* stationary points and *nesting* properties of the spectrum.

2 The calculation

Our calculation follows the general trends described in detail in Ref. [12, 13, 15]. Hamiltonian (2), with periodic boundary conditions, is written in terms of fermion variables (c_j, c_j^\dagger) using the Jordan-Wigner transformation:

$$S_j^x = L_j(c_j + c_j^\dagger)/2, \quad S_j^y = L_j(c_j - c_j^\dagger)/2i, \quad S_j^z = c_j^\dagger c_j - 1/2, \quad (3)$$

with L_j being the sign string that adjusts the anticommutation relations for the (c_j, c_j^\dagger)

$$L_j = \prod_{l=1}^{j-1} (1 - 2c_l^\dagger c_l), \quad L_1 \equiv 1, \quad L_j^2 = 1. \quad (4)$$

For the fermion Hamiltonian (c -Hamiltonian), we solve the *c-cyclic* problem, where one neglects a correction term that comes from the boundary, as it is usually done when studying the thermodynamic limit ($N \rightarrow \infty$) [14]. The *c-cyclic* Hamiltonian is diagonalized in two steps:

i) we take the Fourier transform

$$b_k = \sqrt{\frac{1}{N}} \sum_{j=1}^N c_j \exp(i k j),$$

with $k = 2m\pi/N$ ($-N/2 \leq m \leq N/2 - 1$). At this stage, the Hamiltonian is not diagonal since the anisotropy couples the modes $(k, -k)$;

ii) complete diagonalization is achieved with a Bogoljubov transformation

$$\eta_k = u_k b_k + i v_k b_{-k}^\dagger, \quad \eta_k^\dagger = u_k b_k^\dagger - i v_k b_{-k}, \quad (5)$$

with real coefficients (u_k, v_k) and Hamiltonian

$$\mathcal{H} = \sum_k \hbar \Lambda_k \eta_k^\dagger \eta_k + C, \quad (6)$$

where C is a constant term and the quasi-particle dispersion relation is given by

$$\Lambda_k = 2\omega_J \sqrt{(\gamma \sin k)^2 + (r + \cos k)^2} . \quad (7)$$

In the particle-hole representation, $\Lambda_k \geq 0$ and the ground state is the vacuum for the η operators. We note that the spectrum given by (7) may present a gap as a function of the anisotropy γ and transverse field r . Several examples are available:

- (a) for $\gamma = 1$ (Ising with transverse field), the spectrum presents a gap at $k = \pi$ of magnitude

$$\Delta = 2|1 - r| \quad (8)$$

in units of the exchange constant, which shows that there is a critical value $r_c = 1$ for the transverse field;

- (b) when $r = 0$ (no magnetic field), we get a gap at $k = \pi/2$ whose value is

$$\Delta = 2\gamma , \quad (9)$$

the isotropic XY model being gapless;

- (c) with magnetic field and anisotropy, when $r \leq 1 - \gamma^2$, the gap is positioned at $k = \arccos\left(-\frac{r}{1-\gamma^2}\right)$, with value

$$\Delta = 2\gamma \sqrt{1 - \frac{r^2}{1 - \gamma^2}} . \quad (10)$$

Otherwise, its position and value are given by (8).

Once the ground state and excitations have been determined, we proceed to calculate the dynamical properties of the magnetization. This is done using the identity

$$\langle A \rangle_t = \text{Tr} [\rho(t)A] = \text{Tr} [\rho(0)A(t)] , \quad (11)$$

where $A(t)$ is an operator in the Heisenberg picture. This way, (11) relates the temporal evolution of the average at any time with the initial state $\rho(0)$. We will probe the dynamics of the longitudinal (parallel to the field) Fourier component of the magnetization

$$\langle S_Q^z \rangle_t = \text{Tr} [\rho(t)S_Q^z] = \text{Tr} [\rho(0)S_Q^z(t)] , \quad (12)$$

with

$$S_Q^z \equiv \sum_{j=1}^N S_j^z \exp(i Qj) .$$

Exact closed forms for (12) are obtained when one assumes that the initial density matrix is a functional of only one spatial component of the spins, a situation

that can be achieved in practice using strong non-homogeneous magnetic fields along a given direction, to prepare the initial state [12, 13]. We will denote those possibilities as $\rho(0, S^\mu)$, with $\mu = x, y, z$ labeling the possible field directions. The calculation follows the general trends described in Ref. [13, 15]. The details will be given elsewhere [16]. Note that the calculation of the dynamics of the transverse components S_Q^x and S_Q^y is much more involved, and it is not clear that one can obtain closed analytic formulae. For the above components we only obtained numeric results in small systems.

For the longitudinal component, we summarize the main steps of the calculation below:

- (a) transform S_Q^z to fermion operators to get its time dependence. This step leads to:

$$S_Q^z(t) = -\frac{N}{2}\delta_{Q,0} + \sum_{k=-\pi}^{\pi-2\pi/N} \left\{ \left(u_p u_q e^{i\Omega^- t} \eta_p^\dagger \eta_q + v_p v_q e^{-i\Omega^- t} \eta_{-p}^\dagger \eta_{-q} \right) + \right. \\ \left. + \left(-i u_p v_q e^{i\Omega^+ t} \eta_p^\dagger \eta_{-q}^\dagger + i v_p u_q e^{-i\Omega^+ t} \eta_{-p}^\dagger \eta_q^\dagger \right) \right\} , \quad (13)$$

where $p = k - Q/2$, $q = k + Q/2$, $\Omega^\pm(k, Q) \equiv \Lambda_p \pm \Lambda_q$, and (u, v) are the coefficients in the transformation (5). Note that in (13) there are contributions from processes that do not conserve the number of particles;

- (b) average with the initial density matrix. This means that we have to calculate the averages $\langle \eta_p^\dagger \eta_q \rangle_0$, $\langle \eta_{-p}^\dagger \eta_{-q} \rangle_0$, $\langle \eta_p^\dagger \eta_{-q}^\dagger \rangle_0$, and $\langle \eta_{-p}^\dagger \eta_q^\dagger \rangle_0$ in (13) over the initial state;
- (c) take the thermodynamic limit $N \rightarrow \infty$, *i.e.* introduce an infinite number of degrees of freedom. As a consequence, summations over the k -space are replaced by integrals over the Brillouin zone. Using the symmetry of k , one can reduce the integration to the interval $[0, \pi]$;
- (d) find asymptotic analytic expressions for very long times, $t \rightarrow \infty$.

Note the order of the limiting processes of the two last steps. Indeed, for finite N , the limit $t \rightarrow \infty$ does not exist. We will comment on this further in the following. For the intended scope of this paper, we will just consider the behavior of $\langle S_Q^z \rangle_t$ for the initial ensemble $\rho(0, S^z)$. All the cases, along with complete formulae, are given in [16]. We quote the exact result which comes from taking the continuous limit in (13):

$$\langle S_Q^z \rangle_t = \frac{1}{2\pi} \langle S_Q^z \rangle_0 \int_0^\pi dk \left\{ h(k, Q) \cos[\Omega^-(k, Q) t] + \right. \\ \left. + g(k, Q) \cos[\Omega^+(k, Q) t] \right\} , \quad (14)$$

where the frequencies Ω^\pm are defined above and the functions (h, g) are given by:

$$\begin{aligned} h(k, Q) &\equiv 1 + \frac{(2\omega_J)^2}{\Lambda_p \Lambda_q} [r^2 + 2r \cos k \cos Q/2 + \cos^2 k (\cos^2 Q/2 + \\ &\quad + \gamma^2 \sin^2 Q/2) - \sin^2 k (\sin^2 Q/2 + \gamma^2 \cos^2 Q/2)] , \\ g(k, Q) &\equiv 2 - h(k, Q) . \end{aligned} \quad (15)$$

The frequencies Ω^\pm which appear in (13) and (14), correspond to particle-particle, hole-hole and particle-hole excitation processes that contribute to the time evolution of S_Q^z . Note that for the regime $t \rightarrow \infty$, the integral (14) is strongly oscillatory, and integration over ordinary points leads to cancellations effects (destructive interference). The asymptotic behavior, obtained through the *stationary phase method* [10], is dominated by the contributions of stationary points, where we get constructive interference. The detailed study of stationary points of Ω^\pm depends on γ , r and Q . The points $k = 0$ and $k = \pm\pi$ are always solutions. In addition, the other stationary points are given as roots of a polynomial of fifth degree of the variable $y = \cos k$. This means that the general problem has no analytic solutions, unless a fortuitous factorization is achieved. This way, we have only obtained analytic expressions for two important particular cases: model ii), the Ising model with transverse field ($\gamma = 1$ and arbitrary r); and model iii), no transverse field ($r = 0$) and arbitrary anisotropy γ . As a general rule, the contribution of stationary points leads to an asymptotic relaxation with time in the form of a power law. We write

$$\langle S_Q^z \rangle_t \sim \sum_n J_n^+(t) + \sum_n J_n^-(t) , \quad (16)$$

where (n, \pm) labels the stationary point of Ω^\pm respectively. The number of stationary points and their degeneracy depend only on the parameters of the Hamiltonian (γ, r) and the wave vector Q . The dominant time dependence of the $J_n^\pm(t)$ functions in (16) is given by

$$J_n^\pm(t) = K_n^\pm \exp(i\Theta_n^\pm t) \left(\frac{t}{\tau_n^\pm} \right)^{-\nu_n^\pm} , \quad (17)$$

using the same notation as above. The important quantities in (17) are the relaxation rate τ^\pm and the exponent ν^\pm , which together determine the relative speed of the relaxation process. For the cases we calculated analytically, they are functions of (γ, Q) or (r, Q) . In Fig.1, we display the relaxation times as function of γ for a given value of the wave vector Q (with $r = 0$). The asymptotic behavior is dominated by the contribution of five stationary points of Ω^+ : two of them are related to τ_1 (the points $k = 0, \pi$), a third one ($k = \pi/2$) is associated with τ_2 , and from the two remaining we get the same relaxation time τ_3 . The times τ_2 and τ_3 become asymptotically large in the vicinity of a critical value of γ , which is indicated in the figure, where the corresponding stationary points become degenerate. Some general comments are in order:

- i) the asymptotic behavior oscillates with a small number of frequencies Θ_n^\pm , which are functions of (γ, Q) or (r, Q) ;
- ii) we get a whole set of exponents ν_n^\pm coming from the different stationary points, but the relaxation for $t \rightarrow \infty$ is driven by the smallest exponent ν_0 ;
- iii) depending on their variation in the parameter space, some stationary points may become degenerate. This fact drastically affects the relaxation. As remarked before, the τ 's asymptotically diverge in the neighborhood of critical points. Exactly at the critical values, one has to go some steps further in the asymptotic expansion (as many as the order of the degenerate point), yielding a discontinuous change of the ν_0 exponent. In the example of Fig. 1, the exponent ν_0 changes from $1/2$ to $1/4$ at the critical γ_C , signaling a slowing down of the relaxation process;
- iv) the above instance occurs at the loci of the *critical* curves $Q = Q_C$ in the parameter space, with Q_C given by:

$$Q_C(\gamma = 1, r) = \begin{cases} 2 \arccos r, & r < 1, \\ 2 \arccos(\frac{1}{r}), & r > 1 \end{cases}, \quad (18)$$

for the Ising case with transverse field, and

$$Q_C(\gamma, r = 0) = \arccos\left(\frac{1-\gamma}{1+\gamma}\right), \quad \text{for } 0 \leq \gamma < 1, \quad (19)$$

for the anisotropic case and no field. Note that the gapless cases ($\gamma = 1, r = 1$) and ($\gamma = 0, r = 0$) yield $Q_C \rightarrow 0$, which is an ordinary stationary point. Also note that the pure Ising case ($\gamma = 1, r = 0$) has no dynamics and has to be treated separately.

The above results are exact in infinite chains, where the thermodynamic limit implies a continuous spectrum. In contrast, finite systems present quantum recurrences, with partial or total reconstruction of the initial state. For very small samples, we are able to identify a number of Rabi-like periods associated with the revival of the magnetization. Numerical computations show that those periods or quasi-periods become longer with increasing sizes, scaling almost linearly with N . This poses the question of how to define the time interval during which the finite system approximate the infinite system in a regular way, in the spirit of finite-size scaling methods. To estimate the relaxation, we have adopted the following procedure: *a*) we numerically analyze the dynamics of finite systems until the first partial reconstruction (this time depends on size and γ), and; *b*) we fit the time evolution to a power law similar to the one given by (17). This is not an easy task, since there are several frequencies superimposed. A typical behavior of the magnetization is shown in Fig. 2, for $N = 100$ and for the same Q wave vector of Fig.1. We estimate the exponent from the envelopes of local maxima and minima, which are shown in the figure.

In Fig. 3, we display a summary of our findings for $N = 100$ spins. One observes a precursory slowing down of the relaxation around the critical value predicted for the infinite chain (see Fig. 1), with a typical rounding due to size effects. We comment those results further in the next section.

3 Conclusions

One interesting feature of the anisotropic XY model is the absence of any spin conservation law (we exclude the pure Ising limit without transverse field). This fact makes its dynamics ‘richer’ than the one associated with other models, where the total spin or one of the total spin projections are conserved [12, 13]. This appears as a source of entanglement, which is relevant for applications in quantum computation. Another peculiarity of the XY model is exhibited in (1) and (14), meaning that the dynamics of the longitudinal Fourier component of the magnetization is independent of the initial state, which enters just through a scale factor in the form of an average over the initial condition. This property is not shared by other models, like the Heisenberg XXZ model, where we found a strong dependence of the relaxation process on the initial state [17].

From our analytic and numeric computations, we were able to identify long-lived collective excitations, which have the character of dynamic spin density waves with incommensurate wave vector Q_C . In the vicinity of Q_C , we get $\tau(Q) \rightarrow \infty$ asymptotically, thus reducing the damping of those excitations in relation to a general wave vector Q . Exactly at the point $Q = Q_C$, the exponent ν_0 changes discontinuously ($1/2 \rightarrow 1/4$) and the relaxation time τ has a finite value. Note that *critical* modes only appear when the spectrum has a gap, in agreement with findings in other models of the XY family [11, 12, 13].

Our theoretical results may be physically realized in a number of systems, from which the most promising to perform quantum computation are Josephson tunneling junction arrays. Quantum bits (‘qubits’) stored in low-capacitance Josephson junctions (JJ) simulate mesoscopic spins, and the coupling between JJ units mimic the spin-spin interactions that are usually found in several spin models [4]; in particular one can obtain an effective anisotropic XY coupling with a gap in the spectrum. Nonhomogeneous initial states considered in this paper, could be practically achieved in JJ systems by locally manipulating gate voltages, tunneling barriers or magnetic fields. This way, one may implement exact prescriptions to prepare those long-lived collective excitations as many times as necessary to perform specific tasks in a quantum computer [18]. Those states (which are not stationary states), are obtained by constructive interference from a macroscopically dense number of quantum states. This can be seen from the fact that the degeneracy of stationary points and the critical condition are associated to nesting of the one-particle spectrum around inflection points of the dispersion relation [19]. This peculiarity confers a degree of ‘robustness’ that is still present in finite systems, as shown in our example with $N = 100$, and leads one to expect that quantum coherence will be maintained within operational levels when in contact with the ‘outside world’.

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- [19] Without magnetic field ($r = 0$), inflection points of the dispersion (7) are given at $k = \pm(\pi/2 \pm Q_C/2)$. Around the inflection points the dispersion can be linearized, yielding two pairs of parallel branches (*nesting*). At the critical condition, $Q = Q_C$, we get three stationary points of Ω^+ which are degenerate at $k = \pi/2$. Their contribution to the magnetization (14) is obtained by integrating over nested branches.

FIGURE CAPTIONS

Fig. 1

The inverse of the relaxation times (adimensional units) associated with the stationary points of Ω^+ as a function of γ for the value $Q = 2\pi/5$. They were obtained through the asymptotic behavior at very long time ($t \rightarrow \infty$) of the infinite chain. Here, the wave vector Q is fixed and the anisotropy is varied, crossing through the critical value $\gamma_C = 0.528$, which is indicated by an arrow. At γ_C , two branches are degenerate, and the corresponding relaxation times asymptotically diverge. Note that the branch of τ_3 does not exist for $\gamma > \gamma_C$.

Fig.2

Typical time evolution of the magnetization $\langle S_Q^z \rangle(t)$ in a finite system, for a value of γ away from criticality. The Q wave vector is the same of Fig.1, and the subindex n means that the magnetization is normalized to the initial value at $t = 0$. A regular relaxation behavior is obtained until $\omega_J t \approx 250$, after which we observed the onset of the first partial reconstruction. The exponent of relation (17) is fitted using data from the upper (squares) and lower (circles) envelopes. In the displayed case, we obtained $\nu_0(\text{upper}) \approx 0.476$ and $\nu_0(\text{lower}) \approx 0.482$, which are close to the predicted value $\nu_0 = 1/2$ for the infinite chain.

Fig. 3

The exponent ν_0 from numeric calculations for $N = 100$ spins as a function of the anisotropy parameter γ , for the same Q wave vector of the preceding figures. The analytic calculation for the infinite chain predicts a critical value $\gamma_C = 0.528$, where the exponent ν_0 jumps from $1/2$ to $1/4$. The error bar represents the dispersion obtained from estimating the exponent using the upper and lower envelopes of the relaxation (see Fig. 2).

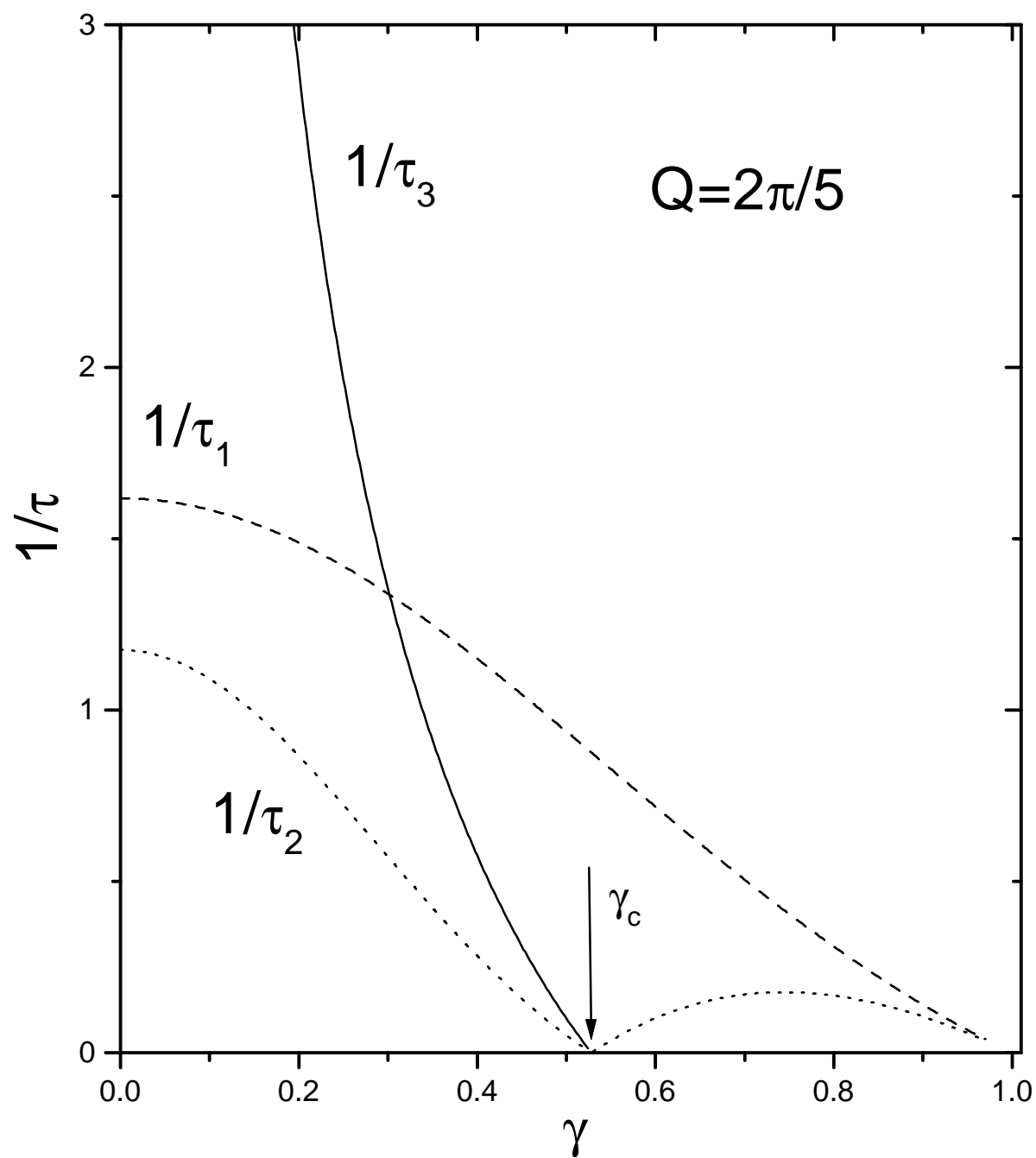


Fig. 1 Phys. Lett. A, Tygel et al.

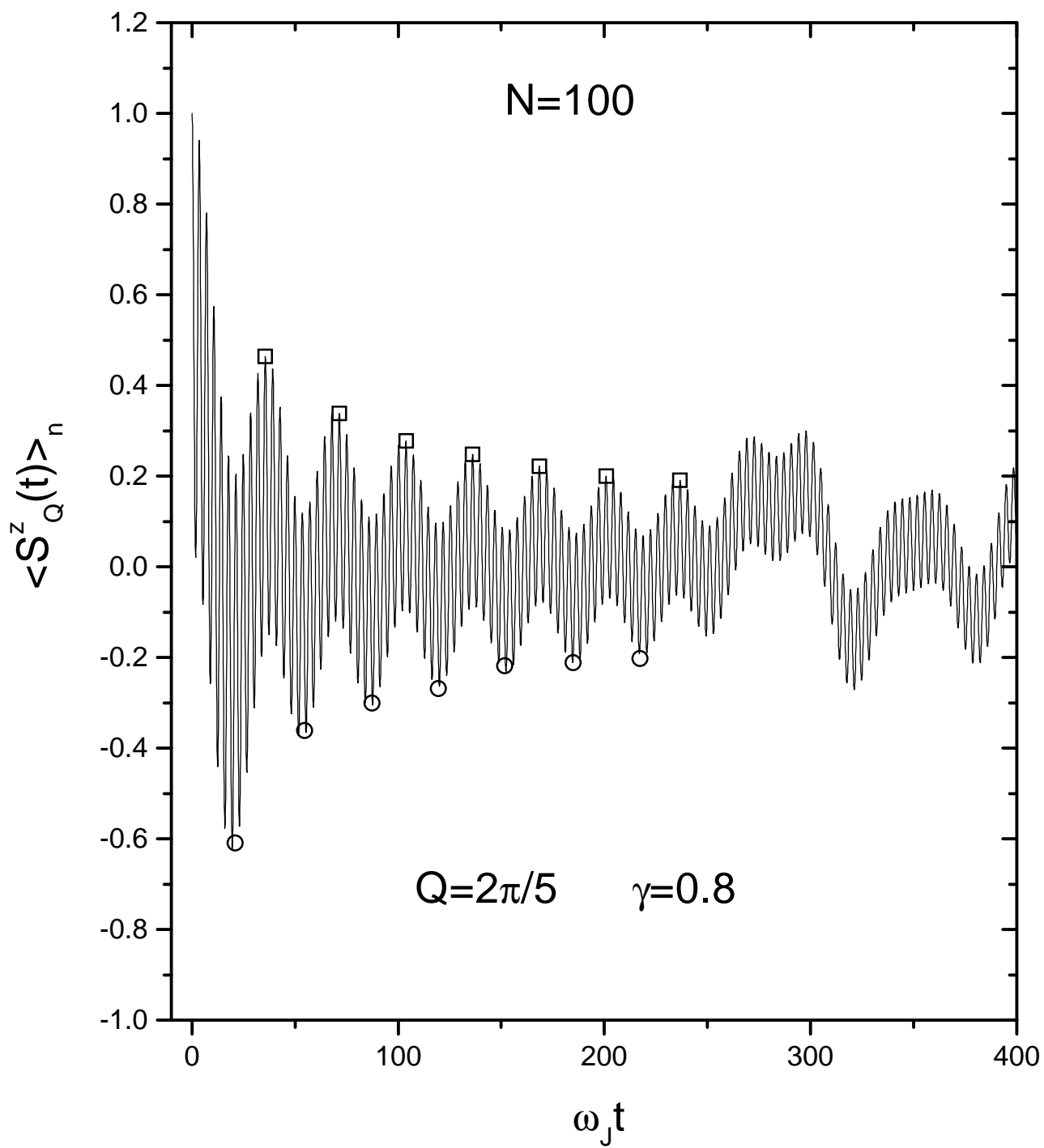


Fig. 2 Phys. Lett. A, Tygel et al.

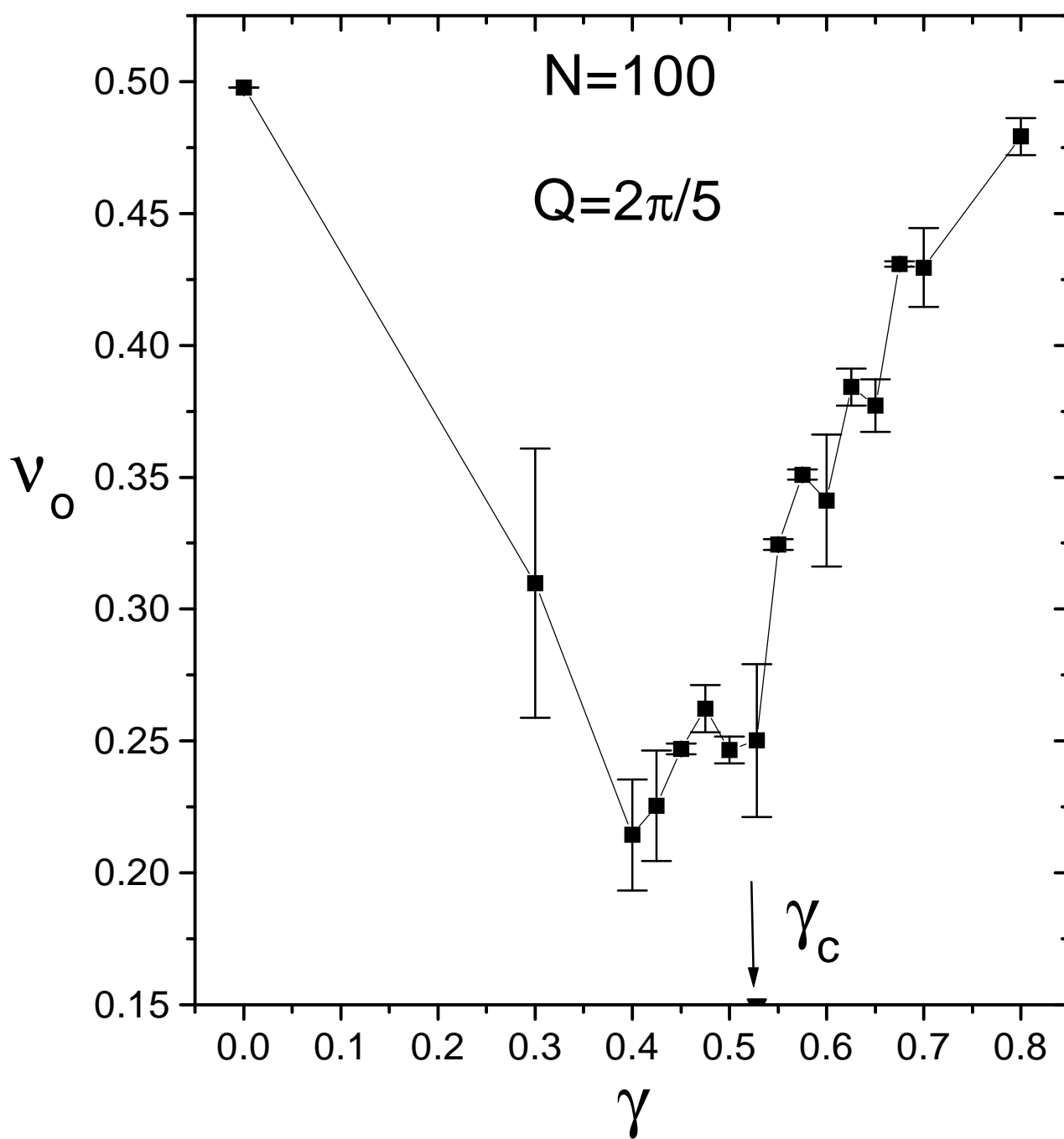


Fig. 3 Phys. Lett. A, Tygel et al.